# High-Order Output-Based Adaptive Methods for Steady and Unsteady Aerodynamics

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# Outline

#### Introduction

- 2 Discretization
- Output error estimation
- Mesh Adaptation
- Unsteady systems
- 6 A hybrid DG discretization
- Concluding remarks

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# Introduction

#### Complex CFD simulations made possible by

- Increasing computational power
- Improvements in numerical algorithms

#### New liability: ensuring accuracy of computations

- Management by expert practitioners is not feasible for increasingly-complex flow fields
- Reliance on best-practice guidelines is an open-loop solution: numerical error is unchecked for novel configurations
- Output calculations are not yet sufficiently robust, even on relatively standard simulations

## Errors in simulations come from various sources



# Verification is important

AIAA Drag Prediction Workshop III (2006)

- Wing-body geometry,  $M = 0.75, C_L = 0.5, Re = 5 \times 10^6$
- Drag computed with various state of the art CFD codes



6/110

# Numerical errors have come down, at a large cost



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# Uniform grid refinement may be misleading

- DPW III wing-alone case:  $M_{\infty} = 0.76, Re = 5 \times 10^6$
- Two mesh sequences generated using best-practice mesh-generation guidelines [Mavriplis, 2007]
- Run on same code (turbulence model, solver, etc)



# Verification = control of numerical error

- Dominant source is discretization error (i.e. lack of appropriate mesh resolution)
- Controlling error means answering
  - How much error is present? (error estimation)
  - How can this error be reduced? (mesh adaptation)
- Possible strategies:

	Error estimation?	Effective adaptation?
Resource exhaustion	No	No
Expert assessment	Maybe	Maybe
Convergence studies	Yes	No
Comparison to experiments	Yes	No
Feature-based adaptation	No	Maybe
Output-based methods	Yes	Yes

#### **Error estimation**

- Error estimates on outputs of interest are necessary for confidence in CFD results
- Mathematical theory exists for obtaining such estimates
- Recent works demonstrate the success of this theory for aerospace applications

#### Mesh adaptation

- Error estimation alone is not enough
- Engineering accuracy for complex aerospace simulations demands mesh adaptation to control numerical error
- Automated adaptation improves robustness by closing the loop in CFD analysis

# A typical output-adaptive result



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# Why not just adapt "obvious" regions?

Fishtail shock in  $M_{\infty} = 0.95$  inviscid flow over a NACA 0012 airfoil



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# The role of high order

- High-order methods: errors converge faster than 2<sup>nd</sup>-order
- Typically choose high-order methods for "smooth" problems, where we expect to see convergence plots that look like:



# Can aero applications benefit from high order?

- Question considered by recent high-order CFD workshops
- Aerospace applications usually have both smooth and singular features (shocks, trailing edges)
- Singularities can limit observed rates



# High-order in mesh adaptation

- Adaptation can isolate singularities with small elements
- In many high-order methods, local p-enrichment is possible
- High-order just becomes another refinement tool for efficiently improving accuracy



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## **Conservation equations**

• PDE:

$$\partial_t \mathbf{u} + \partial_i \mathbf{H}_i(\mathbf{u}, \nabla \mathbf{u}) = \mathbf{0}$$

- $i: 1 \le i \le d$  indexes the spatial dimension d (implied sum)
- $\mathbf{u} \in \mathbb{R}^{s}$  is the state vector
- $\mathbf{H}_i \in \mathbb{R}^s$  is the *i*<sup>th</sup> component of the total flux

$$\mathbf{H}_{i} = \underbrace{\mathbf{F}_{i}(\mathbf{u})}_{\text{inviscid flux}} + \underbrace{\mathbf{G}_{i}(\mathbf{u}, \nabla \mathbf{u})}_{\text{viscous flux}}$$

• The viscous flux is

$$\mathbf{G}_i(\mathbf{u}, \nabla \mathbf{u}) = -\mathbf{K}_{ij}(\mathbf{u})\,\partial_j \mathbf{u}$$

# Solution approximation

Polynomials of order  $p_e$  on each element:

$$\mathbf{u}_{h}(\vec{x}) \approx \sum_{e=1}^{N_{e}} \sum_{n=1}^{N_{p_{e}}} \mathbf{U}_{en} \phi_{en}(\vec{x})$$



 $N_e = \# \text{ of elements}$ 

 $N_{p_e}$  = # of basis fcns on element e

$$n_{i}(\vec{x}) = n^{\text{th}}$$
 basis for of order  $p_{e}$  on  $e$ 

 $p_e$  = approximation order on element e

 $\mathbf{U}_{en}$  = vector of *s* coefficients on *n*<sup>th</sup> basis function on element *e* 

# Weak form

• Multiply the PDE by test functions  $\mathbf{v}_h \in \boldsymbol{\mathcal{V}}_h$  to get

$$\mathcal{R}_h(\mathbf{u}_h,\mathbf{v}_h)=0, \quad orall \mathbf{v}_h \in oldsymbol{\mathcal{V}}_h$$

• Integrating by parts and using BR2, we obtain

$$\mathcal{R}_{h}(\mathbf{u}_{h}, \mathbf{v}_{h}|_{\Omega_{e}}) = \int_{\Omega_{e}} \mathbf{v}_{h}^{T} \partial_{t} \mathbf{u}_{h} d\Omega - \int_{\Omega_{e}} \partial_{i} \mathbf{v}_{h}^{T} \mathbf{H}_{i} d\Omega + \underbrace{\int_{\partial\Omega_{e}} \mathbf{v}_{h}^{+T} \left(\widehat{\mathbf{F}} + \widehat{\mathbf{G}}\right) ds}_{\text{interface/boundary flux}} + \underbrace{\int_{\partial\Omega_{e}} \partial_{i} \mathbf{v}_{h}^{+T} \widehat{\mathbf{K}}_{ij} \left(\mathbf{u}_{h}^{+} - \widehat{\mathbf{u}}_{h}\right) ds}_{\text{adjoint-consistency term}}$$

#### **Fluxes**

- $(\cdot)^+$  = quantity from element interior
- $(\cdot)^-$  = quantity from neighbor element
- $(\cdot)^b$  = quantity defined on a boundary
- $\widehat{(\cdot)}$  = an average quantity on a face
- BR2: unique state on an interior face is  $\hat{\mathbf{u}}_h = (\mathbf{u}_h^+ + \mathbf{u}_h^-)/2$



### **Discrete system**

• Discrete residual on element *e* for *n*<sup>th</sup> test function,

$$\mathbf{R}_{en} \equiv \{\mathcal{R}_h(\mathbf{u}_h, \phi_{en}\mathbf{e}_r)\}_{r=1...s} \in \mathbb{R}^s$$

• We lump all residuals and states into single vectors (size N),

 $\mathbf{R}(\mathbf{U}) = \mathbf{0}$ 



# Verification using a manufactured solution

- How do we know if we coded the discretization correctly?
- Analytical solutions are scarce, especially for RANS
- Let's "make up" a solution,

 $\mathbf{u}(\vec{\mathbf{x}}) = \mathbf{u}^{\text{MS}}(\vec{\mathbf{x}}) = \text{chosen by the user}$ 

 $\bullet~$  Substituting  $\mathbf{u}^{MS}(\vec{\mathbf{x}})$  into the PDE gives a remainder of

$$\mathbf{s}^{\mathrm{MS}} \equiv \partial_t \mathbf{u}^{\mathrm{MS}} + \partial_i \mathbf{H}_i(\mathbf{u}^{\mathrm{MS}}, \nabla \mathbf{u}^{\mathrm{MS}})$$

 $\bullet~$  Using this remainder as a negative source term gives a PDE that  $\mathbf{u}^{\rm MS}$  does satisfy,

$$\partial_t \mathbf{u}^{\mathrm{MS}} + \partial_i \mathbf{H}_i(\mathbf{u}^{\mathrm{MS}}, \nabla \mathbf{u}^{\mathrm{MS}}) - \mathbf{s}^{\mathrm{MS}} = \mathbf{0}$$

# Manufactured solution results for RANS

- Pick a sinusoidal variation,  $\rho^{MS} = a_{\rho} + b_{\rho} \sin(c_{\rho}x + d_{\rho}y)$ , and similarly for the other state components.
- $\bullet\,$  Compute and discretize the source term,  $s^{\rm MS}$
- Does solution on progressively-finer meshes approach **u**<sup>MS</sup>? Check with *L*<sub>2</sub> norm:





## Local sensitivities

 Suppose N<sub>μ</sub> parameters affect our PDE, but we only have one scalar output, J(U):

$$\underbrace{\boldsymbol{\mu}}_{\text{inputs} \in \mathbb{R}^{N_{\mu}}} \to \underbrace{\mathbf{R}(\mathbf{U}, \boldsymbol{\mu}) = 0}_{N \text{ equations}} \to \underbrace{\mathbf{U}}_{\text{state} \in \mathbb{R}^{N}} \to \underbrace{J(\mathbf{U})}_{\text{output (scalar)}}$$

• We are interested in how J changes with  $\mu$ ,

$$rac{dJ}{d\mu} \in \mathbb{R}^{1 imes N_{\mu}} = N_{\mu}$$
 sensitivities

• Brute force approach: perturb each entry in  $\mu$  individually, re-solve the PDE, and measure the perturbation in the output

This is inefficient for large  $N_{\mu}$ 

## The discrete adjoint

• We can efficiently compute sensitivities using a discrete adjoint vector,  $\Psi \in \mathbb{R}^N$ ,

$$\frac{dJ}{d\mu} = \Psi^T \frac{\partial \mathbf{R}}{\partial \mu}$$

• Each entry in  $\Psi$  is the sensitivity of *J* to residual source perturbations in the corresponding entry in **R** 



# The discrete adjoint equation

- Consider a small perturbation  $\delta \mathbf{R}$  to the residual
- The resulting (linearized) state perturbation,  $\delta \mathbf{U}$  satisfies

$$\frac{\partial \mathbf{R}}{\partial \mathbf{U}} \delta \mathbf{U} + \delta \mathbf{R} = 0$$

• Also linearizing the output we have,

$$\delta J = \underbrace{\frac{\partial J}{\partial \mathbf{U}}}_{\text{adjoint definition}} \delta \mathbf{U} = \underbrace{\Psi^T \delta \mathbf{R}}_{\text{adjoint definition}} = -\Psi^T \frac{\partial \mathbf{R}}{\partial \mathbf{U}} \delta \mathbf{U}$$

• Requiring the above to hold for arbitrary perturbations yields the linear *discrete adjoint equation* 

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)^T \Psi + \left(\frac{\partial J}{\partial \mathbf{U}}\right)^T = 0$$

# Adjoints in aerodynamics

Consider flow over an airfoil:



The lift adjoint  $\Psi$  is the sensitivity of lift to residual sources.

We have a solution **U** when  $\mathbf{R} = 0$ 







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Lift= $J(\mathbf{U})$ 

The lift adjoint  $\Psi$  is the sensitivity of lift to residual sources.



The lift adjoint  $\Psi$  is the sensitivity of lift to residual sources.



# Sample steady adjoint solution



# Another steady adjoint solution

RAE 2822, 
$$M_{\infty} = 0.5$$
,  $Re = 10^5$ ,  $\alpha = 1^{\circ}$ 



x-momentum primal state



cons. of x-mom drag adjoint

- Adjoint shares similar qualitative features with primal
- Note wake "reversal" in adjoint solution
- The discrete adjoint solution approximates the continuous adjoint when the discretization is *adjoint consistent*

# **Adjoint verification**

• We can verify the discrete adjoint with a sensitivity analysis,

$$\frac{dJ}{d\alpha} = \boldsymbol{\Psi}^T \frac{\partial \mathbf{R}}{\partial \alpha} + \frac{\partial J}{\partial \alpha}$$

- Compare to finite-difference sensitivity calculation
- Example: NACA 0012 airfoil in Re = 5000 flow



- $\bullet\,$  The discrete adjoint,  $\Psi,$  is obtained by solving a linear system
- This system involves linearizations about the primal solution, U, which is generally obtained first
- When the full Jacobian matrix,  $\frac{\partial \mathbf{R}}{\partial \mathbf{u}}$ , and an associated linear solver are available, the transpose linear solve is straightforward
- When the Jacobian matrix is not stored, the discrete adjoint solve is more involved: all operations in the primal solve must be linearized, transposed, and applied in reverse order
- In unsteady discretizations, the adjoint must be marched backward in time from the final to the initial state

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### **Output error estimation**

We want:  $\delta J = J_H(\mathbf{U}_H) - J(\mathbf{U})$ 

This is the difference between *J* computed with the discrete system solution,  $U_H$ , and *J* computed with the *exact* solution, U

We'll settle for:  $\delta J = J_H(\mathbf{U}_H) - J_h(\mathbf{U}_h)$ This is the difference in *J* relative to a finer discretization (*h*)



# **Fine-space injection**

- The fine space can arise from *h* or *p* refinement
- Define an injection of the coarse state into the fine space



• U<sup>*H*</sup><sub>*h*</sub> will generally not satisfy the fine-space equations,

 $\mathbf{R}_h(\mathbf{U}_h^H) \neq \mathbf{0}$ 

### **Fine-space residuals**

- A finer space (e.g. order enrichment) can uncover residuals in a converged solution
- Example: NACA 0012 at  $\alpha = 2^{\circ}$  in Re = 5000,  $M_{\infty} = 0.5$  flow



## **Fine-space residuals**

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# The adjoint-weighted residual

- $\mathbf{U}_{h}^{H}$  solves a *perturbed* fine-space problem find  $\mathbf{U}_{h}^{\prime}$  such that:  $\mathbf{R}_{h}(\mathbf{U}_{h}^{\prime}) \underbrace{-\mathbf{R}_{h}(\mathbf{U}_{h}^{H})}_{\delta \mathbf{R}_{h}} = 0 \Rightarrow \text{answer: } \mathbf{U}_{h}^{\prime} = \mathbf{U}_{h}^{H}$
- The fine-space adjoint,  $\Psi_h$ , then tells us to expect an output perturbation of

$$\underbrace{J_h(\mathbf{U}_h^H) - J_h(\mathbf{U}_h)}_{\approx \delta J} = \mathbf{\Psi}_h^T \delta \mathbf{R}_h = -\mathbf{\Psi}_h^T \mathbf{R}_h(\mathbf{U}_h^H)$$

- This equation assumes small perturbations (e.g. if nonlinear)
- In summary, we have an *adjoint-weighted residual* error estimate,

$$\delta J \approx - \boldsymbol{\Psi}_h^T \mathbf{R}_h(\mathbf{U}_h^H)$$

# Adjoint-weighted residual example

Fine space residual,  $\mathbf{R}_h(\mathbf{U}_h^H)$ 



Fine space adjoint,  $\Psi_h$ 



Error indicator,  $\epsilon_e = |\mathbf{\Psi}_{h,e}^T \mathbf{R}_{h,e}(\mathbf{U}_h^H)|$ 



Output error:  $\delta J \approx - \Psi_h^T \mathbf{R}_h(\mathbf{U}_h^H)$ 

Idea: adapt where  $\epsilon_e$  is high, to reduce the residual there

### **Two more definitions**

#### **Corrected output**

$$J_H^{\text{corrected}} = J_H - \delta J$$

- Should converge faster than J<sub>H</sub>
- Remaining error = error left in corrected output

#### **Error effectivity**

$$\eta_H = \frac{J_H(\mathbf{U}_H) - J_h(\mathbf{U}_h)}{J_H(\mathbf{U}_H) - J}$$

- J = exact output
- We want  $\eta_H$  close to 1
- Effectivity is affected by choice of fine space

#### **Error convergence tests**

Expect

error = 
$$Ch^k$$
, as  $h \to 0$ 

- *k* = rate of convergence
- *h* = measure of element size (precise value not important)
- For 2D uniform-refinement studies, can use  $h = \sqrt{1/N_e}$
- Taking a log of the above equation,

$$\log(\text{error}) = \log C + k \log \left(\sqrt{\frac{1}{N_e}}\right)$$

• We can measure *k* by plotting log(error) versus log(*h*)

#### Drag error in inviscid flow over a bump



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#### Drag error in viscous flow over an airfoil





# **Error estimation summary**

- Solve the coarse-discretization forward and adjoint problems:  $U_H$  and  $\Psi_H$
- Pick a fine discretization "h" (mesh refinement or order enrichment)
- Solution Calculate or approximate  $\Psi_h$  = adjoint on the fine space
- Project U<sub>H</sub> onto the fine discretization and calculate the residual R<sub>h</sub>(U<sup>H</sup><sub>h</sub>)
- Weight the fine-space residual with the fine-space adjoint to obtain the output error estimate
- The computed output error  $\delta J$  is an estimate of the true error, not a bound

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# **Mesh adaptation**



# **Error localization**

 Recall that the adjoint-weighted residual expression for the output error involves a sum over elements (e)

$$J_H(\mathbf{U}_H) - J_h(\mathbf{U}_h) \approx -\boldsymbol{\Psi}_h^T \mathbf{R}_h(\mathbf{U}_h^H) = -\sum_e \boldsymbol{\Psi}_{he}^T \mathbf{R}_{he}(\mathbf{U}_h^H)$$

• The absolute-value of each element's contribution to the error is the error indicator on that element

$$\epsilon_e \equiv \left| \boldsymbol{\Psi}_{he}^T \mathbf{R}_{he} (\mathbf{U}_h^H) \right|$$

<u>*Right*</u> : plot of error indicator for a viscous DG simulation,  $p_H = 1$ ,  $p_h = 2$ 



# **Output-based mesh adaptation**

#### **Motivating ideas**

- The error indicator (ϵ<sub>e</sub>) identifies elements with large adjoint-weighted residuals
- Locally refining a mesh reduces local residuals
- So we can reduce the output error by refining those elements that have a high  $\epsilon_e$

#### **Adaptation choices**

- Local refinement versus global re-meshing
- Which/how many elements should be targeted?
- Isotropic versus anisotropic refinement
- h, p, or hp mechanics
- Should coarsening be allowed?

# Local mesh modification

- Modify the mesh incrementally (mesh generation is hard)
- Often more robust than global re-meshing
- With node movement, can be flexible for unstructured meshes
- Hanging nodes easily supported in DG



Hanging-node refinement

# **Global re-meshing**

- Entire mesh is re-generated
- Current mesh still plays a role in defining a Riemannian metric
- Useful software in 2D: Bi-dimensional Anisotropic Mesh Generator (BAMG)
- Example of refinement near a single point:



# Incorporating anisotropy

- Crucial for high-Reynolds number simulations, esp. in 3D
- Can come in via a metric or discrete hanging-node "slices"



Anisotropic metric in 2D

choice 2 choice 1 choice 3 = both

Hanging-node choices

- Assess need for anisotropy by
  - Looking at derivatives of a scalar quantity (Mach number)
  - Solving local sub-problems to determine impact of anisotropy directly on the output error

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### Targeting strategies [Nemec et al, 2008]



Constant threshold: refine all elements above a constant error indicator



Decreasing threshold: threshold decreases with each iteration

# **Curved boundaries**

- DG needs an accurate representation of curved boundaries
- Curving elements is not easy
- Tangling is hard to avoid, especially in 3D anisotropic elements





pressure contours p = 2 Euler flow over a linear-element bump representation



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Agglomeration: linear  $\rightarrow$  cubic elements

52/110

# Inviscid flow over an airfoil



- We obtain  $\Psi_h$  approximately (adaptation unaffected)
- Adaptive refinement "quarantines" the trailing edge singularity and uncovers the superconvergent 2p + 1 rate

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# Viscous flow over an airfoil





- Rate in uniform refinement limited by high-order singularities
- Adaptive refinement uncovers a superconvergent rate (2p)

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### Transonic RANS flow over an airfoil





# Transonic RANS flow over an airfoil (ctd.)

- Fine space adjoint solved approximately
- Anisotropic adaptation driven by local solves on discrete refinement choices
- Outputs from uniform refinement overshoot exact values



# Transonic RANS flow over a wing

#### DPW III wing-alone case: $M_{\infty} = 0.76, Re = 5 \times 10^6$

- Initial mesh: cubic hex elements generated by agglomeration of linear multiblock meshes (first element  $y^+ \approx 1$ )
- Artificial viscosity shock capturing
- Spalart-Allmaras turbulence model with negative ν̃ modification [Oliver & Allmaras]
- Drag-adaptive simulation using hp discrete choice algorithm (Ceze + Fidkowski, 2013)



Contours of  $c_p$  and  $\tilde{\nu}$ 

# DPW wing: adapted meshes



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# DPW wing: comparison to uniform refinement



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# DPW wing: comparison to uniform refinement



# Outline

#### Introduction

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# A simple time discretization

Discretizing space only gives

$$\mathbf{M}\frac{d\mathbf{U}}{dt} + \mathbf{R}(\mathbf{U}) = \mathbf{0},$$

where  $\mathbf{M} \in \mathbb{R}^{N \times N}$  is the mass matrix,

$$\mathbf{M}_{ij} = \mathbf{I}_s \int_{\Omega} \phi_i \phi_j \, d\Omega$$

• Discretizing time via backward Euler, we have

$$\underbrace{\mathbf{M} \frac{\mathbf{U}^m - \mathbf{U}^{m-1}}{\Delta t} + \mathbf{R}(\mathbf{U}^m)}_{\text{unsteady residual: } \mathbf{R}^m} = \mathbf{0}$$

m = time node index

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# **Adjoint discretization**

• Unsteady sensitivity chain

$$\boldsymbol{\mu} \to \boxed{\mathbf{R}^m(\mathbf{U}^n, \boldsymbol{\mu}) = \mathbf{0}} \to \mathbf{U}^n \to J(\mathbf{U}^n)$$

Adjoint equation

$$\sum_{m=1}^{N_t} \left( \frac{\partial \mathbf{R}^m}{\partial \mathbf{U}^n} \right)^T \mathbf{\Psi}^m + \left( \frac{\partial J}{\partial \mathbf{U}^n} \right)^T = \mathbf{0}$$

#### Primal unsteady Jacobian

#### Adjoint unsteady Jacobian



Jacobian transpose  $\Rightarrow$  backwards time-marching for the adjoint

# **Discontinuous Galerkin in time**

- Finite element in time: time intervals  $\rightarrow$  "slabs"
- Order *r* temporal representation in each slab
- Spatial order can vary in time (dynamic order)
- End-of-slab solution provides initial condition for the next slab



## **DG-in-time equations**

Multiplying the PDE by temporal test functions  $\varphi_h^m$  and integrating by parts gives (r+1) unsteady residual vectors, enumerated by *m*,

$$\mathbf{R}_{h}^{km} \equiv \underbrace{a^{mn}\mathbf{M}_{h}^{k,k}\mathbf{U}_{h}^{kn} - \varphi_{h}^{m}(t_{k-1})\mathbf{M}_{h}^{k,k-1}\mathbf{U}_{h}^{k-1,r+1}}_{\text{from }d\mathbf{U}_{h}/dt} + \int_{t_{k-1}}^{t_{k}} \varphi_{h}^{m}(t)\mathbf{R}_{h}\left(\mathbf{U}_{h}^{k}(t)\right) dt$$

$$\underbrace{\mathbf{U}_{h}^{k-1,r+1}}_{\text{slab }k-1} + \underbrace{\mathbf{U}_{h}^{k,1}}_{t_{k-1}} + \underbrace{\mathbf{U}_{h}^{k}(t)}_{t_{k-1}} + \underbrace{\mathbf{U}_{h}^$$

# **DG-in-time adjoint**

- Total number of time nodes:  $N_t = N_k(r+1)$
- $\Psi_H^{km}$  = the adjoint at time slab *k*, time node *m*
- Unsteady adjoint equation

$$\underbrace{\left(\frac{\partial \mathbf{R}_{h}^{km}}{\partial \mathbf{U}_{h}^{ln}}\right)^{T} \mathbf{\Psi}_{h}^{km} + \left(\frac{\partial J_{h}}{\partial \mathbf{U}_{h}^{ln}}\right)^{T}}_{\mathbf{R}_{\psi h}^{ln}(\mathbf{\Psi}_{h}^{km})} = 0$$

k, l =time slab indices m, n =intra-slab time node indices

Primal and adjoint systems can both be solved using a relatively cheap, inexact Newton method

## **Output error estimation**

• The adjoint-weighted residual extends to unsteady systems,

$$\delta J \approx -\Psi_h^T \mathbf{R}_h(\mathbf{U}_h^H) = -\sum_{k=1}^{N_k} \sum_{m=1}^{r+1} \left(\Psi_h^{km}\right)^T \mathbf{R}_h^{km}(\mathbf{U}_h^H)$$
$$= -\sum_{k=1}^{N_k} \sum_{e=1}^{N_e} \sum_{\substack{m=1\\e=1}}^{r+1} \left(\Psi_{he}^{km}\right)^T \mathbf{R}_{he}^{km}\left(\mathbf{U}_h^H\right)$$
$$= -\sum_{k=1}^{N_k} \sum_{e=1}^{N_e} \sum_{\substack{m=1\\e=1}}^{r+1} \left(\Psi_{he}^{km}\right)^T \mathbf{R}_{he}^{km}\left(\mathbf{U}_h^H\right)$$

• The error indicator for element *e* of time slab *k* is

$$\epsilon_e^k = \left| \varepsilon_e^k \right|$$

• Sometimes also interested in a "conservative" error estimate

sum of indicators 
$$= \epsilon = \sum_{k=1}^{N_k} \sum_{e=1}^{N_e} \epsilon_e^k$$

# Space-time anisotropy measure

How much of the error is due to the spatial versus the temporal discretization?












# Space-time error indicators

- One can use the projection-based anisotropy measure on each space-time element
- These projections give separate  $\varepsilon_{e,k}^{\text{space}}$  and  $\varepsilon_{e,k}^{\text{time}}$  estimates, which then yield spatial and temporal error fractions,

$$\beta_e^{k,\text{space}} = \frac{|\varepsilon_e^{k,\text{space}}|}{|\varepsilon_e^{k,\text{space}}| + |\varepsilon_e^{k,\text{time}}|}, \qquad \beta_e^{k,\text{time}} = 1 - \beta_e^{k,\text{space}}$$

• Adaptive indicators use total space-time error,  $\epsilon_e^k = |\varepsilon_e^k|$ 

spatial indicator on space-time elem  $e, k = \epsilon_e^{k, \text{space}} = \epsilon_e^k \beta_e^{k, \text{space}}$ total spatial indicator on spatial elem  $e = \epsilon_e^{k, \text{space}} = \sum_k \epsilon_e^k \beta_e^{k, \text{space}}$ total temporal indicator on time slab  $k = \epsilon_e^{k, \text{time}} = \sum_k \epsilon_e^k \beta_e^{k, \text{time}}$ 

# Adaptive solution process



- Use bisection of time slabs if just refining
- If also coarsening, need to shuffle all time slabs
- Shuffle using a one-dimensional metric-based algorithm
- Example: refine blue slabs, coarsen gold slabs



# Static spatial refinement

- As a simplification, let's first keep the spatial refinement constant in time
- On each adaptive iteration we *h*-refine some spatial elements
- This is surprisingly efficient for many problems



## Static *h*-refinement, impulsively-started airfoil



# Impulsively-started airfoil: output convergence

Consider space-time refinement using various error indicators



- Acoustic waves distract the unweighted residual indicator
- Local approximation error refinement performs well
- Output-based refinement is the most efficient in DOFs

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# Impulsively-started airfoil: adapted spatial meshes

- Meshes shown at iterations with similar total dofs
- Spatially-marginalized output error estimate  $\epsilon_e$  is shown on the elements of the output-adapted mesh



# Impulsively-started airfoil: adapted time slabs



- Output indicator yields a fairly-uniform temporal refinement
- Approximation error focuses on the initial time (dynamics of the IC) and the latter 1/3 of the time, when the shed vortices develop
- Residual creates a mostly-uniform temporal mesh as it tracks acoustic waves

# Deformable domains

#### ALE Idea: solve transformed PDE on a static reference domain







#### Key definitions

- $\vec{X}$ reference-domain coordinates
- $\vec{x}$ = physical-domain coordinates
- determinant of Jacobian matrix  $\vec{F}$  = physical flux vector g
- $\vec{v}_G$ = arid velocity,  $\partial \vec{x} / \partial t$

- **u** = physical state
- $\mathbf{u}_X$  = reference state
- Ēx reference flux vector

# Analytical motion technique

- Simple and quite general approach for deforming domains
- Near-field rigid body motion blends into a static farfield mesh
- Blending occurs via polynomial functions in the radial coordinate



High-Order Output-Based Adaptive Methods for Steady and Unsteady Aerodynamics K.J. Fidkowski 77/110

# Geometric conservation law (GCL)

- The ALE approach does not guarantee conservation:
  - Cannot always represent a constant physical solution
  - Time integration errors affect conservation
- A GCL by Persson et al (2009) relies on approximating  $\mathbf{u}_{\bar{X}} = \bar{g}\mathbf{u}$  and solving an additional equation

$$\frac{\partial \bar{g}}{\partial t} - \nabla_X \cdot (g\mathcal{G}^{-1}\vec{v}_G) = 0$$

- This equation is local and cheap to solve, but ...
  - We need to integrate with higher quadrature rules
  - We now need to compute a GCL adjoint for error estimation

# Pitching and plunging airfoils

Consider two airfoils pitching and plunging in series

$$Re = 1200, M_{inf} = 0.3, Str = 2/3, A_{pitch} = \pm 30^{\circ}, A_{plunge} = 0.25c$$



**Output**: Lift on the right airfoil integrated from t = 7.25 to 7.5 (the final time)



# Adapted mesh

#### Output-based method

- Targets vortex shedding and larger elements near motion regions
- Refines earlier times, as well as final times over which output is integrated

#### Residual-based method

- Only adapts initial times
- Is again distracted by acoustic waves



### **Output convergence versus DOF**



### **Output convergence versus CPU time**



# GCL adjoint

To see what's (in part) driving the adaptation, we look at contours of the GCL adjoint. Black and white regions indicate large output sensitivity.



- The output is very sensitive to initial vortex shedding from the first airfoil
- Acoustic rings and a convection path between the airfoils indicate two different modes of error propagation

High-Order Output-Based Adaptive Methods for Steady and Unsteady Aerodynamics K.J. Fidkowski 83/110

# **Three-dimensional flapping**

We apply the adaptive strategy to a 3D flapping simulation

 $Re = 500, M_{inf} = 0.3, Str = 0.4, A_{stroke} = \pm 30^{\circ}, A_{pitch} = \pm 10^{\circ}$ 

Case parameters

- Farfield at 20+ chords
- DG1 time scheme
- The order *p* is kept between 0 and 5
- $f_{growth} = 30\%$

•  $f_{coarsen} = 5\%$ 



Wing geometry and kinematics

Output: Lift integrated over final 5% of simulation time

## Adapted spatial meshes

Orders (0 to 3) plotted on entropy isosurfaces for two snapshots of the flow.



### **Output convergence versus DOF**



### Output convergence versus CPU time



# Outline

#### Introduction

- 2 Discretization
- Output error estimation
- 4 Mesh Adaptation
- 5 Unsteady systems
- 6 A hybrid DG discretization
  - 7 Concluding remarks

# Hybridizing DG

In hybrid/mixed DG methods, we introduce *additional* unknowns on faces  $(\hat{u})$ , with the intent that these will be the only globally-coupled unknowns.



# **Motivation: DOF count**

The numbers in the below tables indicate approximately how many degrees of freedom (per equation of a system) we need per vertex of a typical mesh.

Triangles:				Quadrilate	erals:		
method	p = 1	p = 2	p = 3	method	p = 1	p = 2	p = 3
DG	6	12	20	DG	4	9	16
CG	1	4	9	CG	1	4	9
HDG	6	9	12	HDG	4	6	8
EDG	1	4	7	EDG	1	3	5
Tetrahedra	a:			Hexahedra	a:		
Tetrahedra method	p = 1	p = 2	<i>p</i> = 3	Hexahedra method	a:   p = 1	p = 2	<i>p</i> = 3
Tetrahedra method DG	p = 1 24	<i>p</i> = 2 60	<i>p</i> = 3 120	Hexahedra method DG	a: $p = 1$ 8	<i>p</i> = 2 27	$\frac{p=3}{64}$
Tetrahedra method DG CG	p = 1 24 1	p = 2 60 8.2	p = 3 120 27.4	Hexahedra method DG CG	a: $p = 1$ 8 1	<i>p</i> = 2 27 8	p = 3 64 27
Tetrahedra method DG CG HDG	$ \begin{array}{c}     p = 1 \\     \hline         24 \\         1 \\         36 \end{array} $	p = 2 60 8.2 72	p = 3 120 27.4 120	Hexahedra method DG CG HDG	a: p = 1 8 1 12	p = 2 27 8 27	p = 3 64 27 48

# **HDG discretization**

### Introduce $\vec{q}$ to obtain a system of PDEs

$$\begin{array}{lll} \vec{q} - \nabla u &= & \mathbf{0} \\ \partial_t u + \nabla \cdot \underbrace{\left[\vec{F}(u) + \vec{G}(u, \vec{q})\right]}_{\vec{H}(u, \vec{q})} &= & \mathbf{0} \end{array}$$

Trial functions	Test functions	Space
u	W	$\mathcal{V}_h$
$\vec{\mathbf{q}}$	$\vec{\mathbf{v}}$	$[\mathcal{V}_h]^d$
û	$\mu$	$\mathcal{M}_h$

(on elements)  $\mathcal{V}_h = \{ \mathbf{u} \in L^2(\Omega) : \mathbf{u}|_{\Omega_e} \in \mathcal{P}^{p_e}(\Omega_e) \ \forall \ \Omega_e \in T_h \}$ (on faces)  $\mathcal{M}_h = \{ \widehat{\mathbf{u}} \in L^2(\mathcal{E}_h) : \widehat{\mathbf{u}}|_{\sigma_f} \in \mathcal{P}^{p_f}(\sigma_f) \ \forall \ \sigma_f \in \mathcal{E}_h \}$ 

# HDG discretization (ctd.)

#### System of PDEs

$$\begin{aligned} \vec{q} - \nabla u &= 0 \\ \partial_t u + \nabla \cdot \vec{H}(u, \vec{q}) &= 0 \end{aligned}$$

#### Weak form

$$\begin{aligned} (\vec{\mathbf{q}}, \vec{\mathbf{v}})_{T_h} + (\mathbf{u}, \nabla \cdot \vec{\mathbf{v}})_{T_h} - \langle \widehat{\mathbf{u}}, \vec{\mathbf{v}} \cdot \vec{n} \rangle_{\partial T_h} &= \mathbf{0}, \quad \forall \vec{\mathbf{v}} \in [\mathcal{V}_h]^d \\ (\partial_t \mathbf{u}, \mathbf{w})_{T_h} - \left(\vec{\mathbf{H}}, \nabla \mathbf{w}\right)_{T_h} + \left\langle \widehat{\vec{\mathbf{H}}} \cdot \vec{n}, \mathbf{w} \right\rangle_{\partial T_h} &= \mathbf{0}, \quad \forall \mathbf{w} \in \mathcal{V}_h \\ \left\langle \widehat{\vec{\mathbf{H}}} \cdot \vec{n}, \boldsymbol{\mu} \right\rangle_{\partial T_h \setminus \partial \Omega} &= \mathbf{0}, \quad \forall \boldsymbol{\mu} \in \mathcal{M}_h \end{aligned}$$

$$(\mathbf{u}, \mathbf{w})_{T_h} = \sum_{e=1}^{N_e} \int_{\Omega_e} \mathbf{u}^T \mathbf{w} \, d\Omega \qquad \langle \mathbf{u}, \vec{\mathbf{v}} \cdot \vec{n} \rangle_{\partial T_h} = \sum_{e=1}^{N_e} \int_{\partial \Omega_e} \mathbf{u}^{+T} \vec{\mathbf{v}}^+ \cdot \vec{n}^+ \, ds$$

# **HDG fluxes**



- Note, fluxes are one-sided: element-interior degrees of freedom are not directly coupled
- Stabilization borrows ideas from DG (e.g. Rusanov, Roe)

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# **HDG** approximation

inside element 
$$\Omega_e$$
:  $\mathbf{q}(\vec{x})|_{\Omega_e} = \sum_{i=1}^d \sum_{n=1}^{N_{p_e}} \mathbf{Q}_{ein} \phi_n(\vec{x}) \hat{x}_i$   
inside element  $\Omega_e$ :  $\mathbf{u}(\vec{x})|_{\Omega_e} = \sum_{n=1}^{N_{p_e}} \mathbf{U}_{en} \phi_n(\vec{x})$   
on face  $f$ :  $\hat{\mathbf{u}}(\vec{s})|_{\sigma_f} = \sum_{n=1}^{N_{p_f}} \mathbf{A}_{fn} \mu_n(\vec{s})$ 

- **q** and **u** are approximated with the same basis and order, *p<sub>e</sub>* on element *e*
- $\hat{\mathbf{u}}$  is approximated with order  $p_f$  on face f
- $\bullet\,$  The only globally-coupled unknown vector will be  $\Lambda\,$

## Residuals

Three types of residuals: two types inside an element, and one type on interior faces,

$$\begin{aligned} \mathbf{R}_{ein}^{Q} &= \int_{\Omega_{e}} \mathbf{q}_{i} \phi_{n} \, d\Omega + \int_{\Omega_{e}} \mathbf{u} \partial_{i} \phi_{n} \, d\Omega - \int_{\partial\Omega_{e}} \widehat{\mathbf{u}} \phi_{n} n_{i} \, ds \\ \mathbf{R}_{en}^{U} &= \int_{\Omega_{e}} \partial_{t} \mathbf{u} \phi_{n} \, d\Omega - \int_{\Omega_{e}} \vec{\mathbf{H}} \cdot \nabla \phi_{n} \, d\Omega + \int_{\partial\Omega_{e}} \widehat{\mathbf{H}} \cdot \vec{n} \phi_{n} \, ds \\ \mathbf{R}_{fn}^{\Lambda} &= \int_{\sigma_{f}} \left\{ \widehat{\mathbf{H}} \cdot \vec{n} \big|_{L} + \widehat{\mathbf{H}} \cdot \vec{n} \big|_{R} \right\} \mu_{n} \, ds \end{aligned}$$

Note, the integrand appearing in  $\mathbf{R}^{\Lambda}$  can be re-written as

$$\widehat{\mathbf{H}} \cdot \vec{n}\big|_{L} + \widehat{\mathbf{H}} \cdot \vec{n}\big|_{R} = \left[\widehat{\mathbf{H}}(\widehat{\mathbf{u}}, \vec{\mathbf{q}}_{L}) - \widehat{\mathbf{H}}(\widehat{\mathbf{u}}, \vec{\mathbf{q}}_{R})\right] \cdot \vec{n}_{L} + \mathbf{S}_{L}(\mathbf{u}_{L} - \widehat{\mathbf{u}}) + \mathbf{S}_{R}(\mathbf{u}_{R} - \widehat{\mathbf{u}})$$

 $\Rightarrow$  the last set of equations is a weak statement of flux continuity

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### HDG residual Jacobian matrix



## Static condensation



- Let  $\mathbf{Q}\mathbf{U} = [\mathbf{Q}, \mathbf{U}]^T$
- $\mathbf{A} = \frac{\partial \mathbf{R}^{\mathcal{Q}}}{\partial \mathcal{Q}U}$  is easily invertible (element-local solves)
- Define a Schur-complement system matrix as

$$\mathbf{K} = \mathbf{D} - \mathbf{C}\mathbf{A}^{-1}\mathbf{B}$$

## Static condensation (ctd.)

• At each Newton update, we need to solve the system

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \begin{bmatrix} \Delta \mathbf{Q} \mathbf{U} \\ \Delta \mathbf{\Lambda} \end{bmatrix} + \begin{bmatrix} \mathbf{R}^{\mathcal{Q} \mathcal{U}} \\ \mathbf{R}^{\mathbf{\Lambda}} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

• Apply static condensation: i.e. hypothetically solve for QU from the first block and substitute into the second block,

$$\mathbf{K} \Delta \mathbf{\Lambda} + \underbrace{\mathbf{R}^{\Lambda} - \mathbf{C} \mathbf{A}^{-1} \mathbf{R}^{QU}}_{\widetilde{\mathbf{R}}^{\Lambda}} = \mathbf{0}$$

• Solve this (hopefully small) system for  $\Delta \Lambda$ , and then back-substitute to get  $\Delta QU$ 

$$\Delta \mathbf{Q}\mathbf{U} = -\mathbf{A}^{-1}(\mathbf{B}\Delta\mathbf{\Lambda} + \mathbf{R}^{\mathbf{Q}\mathbf{U}})$$
# **Adjoint discretization**

• The adjoint system for output *J* is obtained by using the transpose of the primal Jacobian,

$$\begin{bmatrix} \mathbf{A}^T & \mathbf{C}^T \\ \mathbf{B}^T & \mathbf{D}^T \end{bmatrix} \begin{bmatrix} \mathbf{\Psi}^{QU} \\ \mathbf{\Psi}^{\Lambda} \end{bmatrix} + \begin{bmatrix} \frac{\partial J}{\partial \mathbf{QU}}^T \\ \frac{\partial J}{\partial \mathbf{\Lambda}}^T \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}$$

 Statically condensing out the element-interior degrees of freedom, we obtain the following system for the face adjoints,

$$\underbrace{\begin{bmatrix} \mathbf{D}^T - \mathbf{B}^T \mathbf{A}^{-T} \mathbf{C}^T \end{bmatrix}}_{\mathbf{K}^T} \mathbf{\Psi}^{\Lambda} + \begin{bmatrix} \frac{\partial J}{\partial \mathbf{\Lambda}}^T - \mathbf{B}^T \mathbf{A}^{-T} \frac{\partial J}{\partial \mathbf{Q} \mathbf{U}}^T \end{bmatrix} = \mathbf{0}$$

• Same solution procedure as primal: solve for  $\Psi^{\Lambda}$  first, then for  $\Psi^{QU}$ 

# Error estimation and adaptation

 The adjoint-weighted residual output error estimate applies to an HDG discretization,

$$\delta J \approx \underbrace{-(\boldsymbol{\Psi}_{h}^{Q})^{T} \mathbf{R}_{h}^{Q}}_{\delta J^{Q}} \underbrace{-(\boldsymbol{\Psi}_{h}^{U})^{T} \mathbf{R}_{h}^{U}}_{\delta J^{U}} \underbrace{-(\boldsymbol{\Psi}_{h}^{\Lambda})^{T} \mathbf{R}_{h}^{\Lambda}}_{\delta J^{\Lambda}}$$

- Fine space = order increment on all elements and faces
- All residuals are evaluated using the coarse state injected into the fine space
- $\delta J^{\Lambda}$  is typically very small (sometimes zero)
- We only adapt on localizations of  $\delta J^Q$  and  $\delta J^U$

# Inviscid flow over an airfoil



Mach contours (0-0.6)

Final drag-adapted mesh for p = 2

- Compare adaptive refinements of DG and HDG
- Solve for  $\Psi_h$  approximately using block-Jacobi smoothing

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# Inviscid flow over an airfoil: results



- In HDG,  $\delta J^{\Lambda} = 0$  exactly in this case
- Results nearly identical between HDG and DG
- For high orders, HDG has an advantage of smaller global systems

# **RANS-SA flow over an airfoil**



Mach contours (0–0.6)

Final drag-adapted mesh

- Compare adaptive refinements of DG and HDG
- For solver robustness, the initial mesh is already tailored to resolve the boundary layer

### **RANS-SA flow over an airfoil: results**



# Scalar advection-diffusion

#### Scalar advection diffusion in a box, Pe = 50, Dirichlet BCs





Scalar solution

Final output-adapted mesh

- Output is the heat flux integral on the right boundary
- Compare adaptive refinements of DG and HDG

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K.J. Fidkowski

### Scalar advection-diffusion: results



- DG and HDG now give different results
- Mixed formulation in HDG converges heat flux faster
- Output-adaptation buys an extra order of convergence when considering corrected values

# Outline

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#### Concluding remarks

# **Concluding remarks: summary**

- Presented ideas, methods, and results for output-based adaptive aerodynamics simulations
- Used a discontinuous Galerkin (DG) finite element method for convective stability, *hp* adaptation
- Showed one way to address the cost of DG: hybridization
- Extended adjoint-weighted residual to unsteady and hybridized discretizations
- Showed results for 2D and 3D simulations of compressible flow, including cases with viscosity and Reynolds-averaged turbulence

# Concluding remarks: key findings

- Adjoint error estimates improve robustness of CFD
- Output-based adaptation can quarantine singularities and recover optimal convergence rates
- For many steady problems, output-based adaptation saves DOFs and CPU time compared to uniform refinement or heuristic indicators
- Adaptation mechanics can be tricky, especially with curved anisotropic elements
- Unsteady problems add time as a dimension, and this generally helps adaptation
- Hybrid DG discretizations can reduce globally coupled DOFs at moderate-to-high orders

- Students and post-docs
- Collaborators
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— Thank you —